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CREATIVE RESEARCH ENTERPRISES
In Astrophysics, Atmospheric Physics & Space Sciences

Astrophysics Report # 1

FINAL REPORT ON LMSC P. O. # SCPDE5620,1,2F
(Parent NASA Contract # NASW-4638)

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FINAL REPORT ON LMSC PURCHASE ORDER # SCPDE5620, 1, 2F
(PARENT NASA CONTRACT # NASW-4638)

ABSTRACT

This final report represents the completion of the three tasks under the purchase order # SCPDE5620,1,2F. Chemical composition of gravitationally contracting, but otherwise quiescent, interstellar clouds and of interstellar clouds traversed by high velocity shocks, were modeled in a comprehensive manner that represents a significant progress in modeling these objects. The evolutionary chemical modeling, done under this NASA contract, represents a notable advance over the "classical" fixed condition equilibrium models because the evolutionary models consider not only the chemical processes but also the dynamical processes by which the dark interstellar clouds may have assumed their present state. The shock calculations, being reported here, are important because they extend the limited chemical composition derivable from dynamical calculations for the total density and temperature structures behind the shock front. In order to be tractable, the dynamical calculations must severely simplify the chemistry. The present shock calculations take the shock profiles from the dynamical calculations and derive chemical composition in a comprehensive manner. The results of the present modeling study are still to be analyzed with reference to astronomical observational data and other contemporary model predictions. As far as humanly possible, this analysis will be continued with CRE's (Creative Research Enterprises's) IR&D resources, until a sponsor is found.

1. PREAMBLE:

The work done under the present LMSC P.O. SCPDE5620,1,2F is an extension of the work that was sponsored by NASA's ISR Astronomy program with a grant NAGW-1797 to the University of Southern California. This research effort was later transferred to Lockheed under the contract NASW-4638. The themes of the research were twofold (i) study evolutionary models of chemistry in quiescent dark interstellar clouds, and (ii) elucidate chemical compositions of interstellar clouds perturbed by high velocity shocks. High velocity shocks may behave as the classical J-shock with an abrupt "jump" of physical properties at the shock fronts.

The work being reported here represents the completion of the originally proposed modeling studies, in general, and of the modeling required under the LMSC P.O., in particular. The completion of these modeling studies is also a notable advance. This will be explained in the concluding remarks.

2. DESCRIPTION OF THE WORK DONE:

Work done for Tasks 1 & 2 in the LMSC P.O. will now be described. (Writing of this description was the third task.)

2.1 Task 1 - Chemistry behind J-shocks:

Two model interstellar clouds were considered; one had a density of 10^3 hydrogen nuclei cm^{-3} while the other had a density of 10^5 cm^{-3} . Each cloud was assumed to have been traversed by high velocity shocks moving at speeds of 40 km/s and 80 km/s. These high velocities were selected in order to ensure that the assumption of J-shocks apply, i.e., there is a discontinuous "jump" of physical properties at the shock front. High velocity shock models are appropriate for studying the shock waves driven by high energy phenomenon such as supernova explosions. The task was to determine the chemical compositions behind the shock front.

The chemistry modeling used the distributions of the density, gas and grain temperatures and the far-uv radiation field intensities behind the shock front derived from dynamical calculations done by Dr. Hollenbach of NASA-Ames research Center and his collaborators at UC Berkeley. These quantities were provided as functions of time since the shock hit the cloud (or distance from the shock front). The kinetic temperature reaches very high values for shocks of 40 to 80 km/s. For example, in a cloud of 10^3 cm^{-3} density the temperature just behind the shock front rises to more than 300,000 K. At these high temperatures, impact ionization and

dissociations become quite important, and chemical reactions with significant activation energies also proceed rapidly.

For this Task 1, therefore, the library of chemical reactions used by CRE's investigator in his earlier studies of cold clouds was expanded to incorporate endothermic reactions including the impact dissociation and ionization, and also additional photo-dissociations/photoionizations due to the far-uv emanating from the shock front. This was one of the most demanding part of the total effort which included exacting literature search and integration of about 500 additional reactions into the existing library without any error at all.

Two groups of reactions needed special treatments. Endothermic reactions between neutral (uncharged) atoms or molecules belong to the first group. Laboratory studies of these reactions are done at pressures which ensure local thermal equilibrium (LTE) amongst the translational, vibrational and rotational degrees of freedom. In interstellar clouds, under study here, with densities of at best 10^7 cm^{-3} , the vibrational and translational degrees of freedom may not be in equilibrium. This non-LTE condition significantly affects the rates of endothermic reactions. Rates of several reactions, such as the reactions:



were modified through subroutines that keep doing so during the computations as the conditions of temperatures and densities change. The modification followed the formulae described by Hollenbach and McKee (Ap. J., 342, 306, 1989). The second group of reactions needing special treatment are the electron-ion recombination reactions. Due to quite efficient collisional ionization and ionization by the intense far-uv from the shock front, the electron densities in region close to the shock front approached the total density and the gas becomes almost fully ionized. Under these conditions the electron-ion recombination rates are also greatly affected and need special treatment. In the present study the treatment described by Hollenbach and McKee was followed. Hollenbach and McKee's prescription was followed in order to ensure consistency between their dynamical and the present chemical modeling.

Sulfur bearing molecules were amongst those interstellar molecules that stimulated the early studies of shocked dense clouds. The present studies, therefore, included sulfur compounds,

even though they were excluded in the dynamical models. Polycyclic aromatic hydrocarbons (PAHs) are now considered very important constituents of the interstellar clouds. An important consequence of their presence is that they help to increase the abundance of atomic carbon. Thus, they were also included in the present shock models.

The shock calculations were run in different modes. The first step was to validate the model runs in terms of their meeting several basic criteria of correct numerical algorithms and accuracy. Thus, it was verified that the models conserve charge and mass, and that the predicted abundances of the various species have reached a level of accuracy consistent with the observational data. This was done by varying those parameters in the stiff equation solver routine that control the relative accuracy and absolute accuracies. The results from the present modeling are correct up to a relative accuracy of 1 in 10^4 , and absolute abundances are reliable down at least to 10^{-16} of the total density or across 18 orders of magnitudes.

2.1.2 Preliminary Results:

A vast amount of model data has been generated which will take a long time to thoroughly analyze with respect to comparison with observational data and with the results from other contemporary models. However, it is quite obvious, even now, that we can look forward to a very productive analysis. To illustrate this point, Table 1 compares the results from the dynamical calculations with limited chemistry and the full chemical calculations using the shock structure from the dynamical calculations.

Two points emerge quite clearly. First, even though the sum of all silicon bearing species (just as an example) was the same in the two calculations, the distributions in the various species was very different. This underscores the need of more comprehensive chemical models than are usually done in dynamical models. The fact that the densities of the predominant coolers C, C⁺, CO and H₂O are different in the two calculations is extremely important, because this difference will certainly affect the basic shock profile. This difference is due to differences in the reaction rate coefficients. It could also be due to the simplifications in the chemistry that was made by the dynamical calculations. At the present time we do not know which of the reasons are responsible for the difference. CRE plans to investigate this issue in cooperation with Dr. Hollenbach. If it is discovered that the differences in the densities of the various coolants, then the dynamical calculations

for the shock structure must be done iteratively with the detailed chemical calculations.

Table 1. Comparison of the abundances from the dynamical models with limited chemistry and the full chemical model of a model interstellar cloud with initial density of 10^5 cm^{-3} traversed by a 40 km s^{-1} shock wave

Species densities at $4.3 \cdot 10^5 \text{ s}$	Densities in the dynamical model with limited chem- istry	Densities in the full chemical model
H	3.03e6	3.45e6
C	3.12e2	8.66e1
H ₂	1.35e6	1.15e6
CO	1.01e3	1.23e3
H ₂ O	4.27e1	1.00e2
Si	2.45e-4	1.41e-4
Si ⁺	7.30e-4	1.63e-4
SiO	2.07e1	2.57e-1
HSiO ⁺	2.94e-3	8.52e-5
OH	2.03e0	9.49e0
C ⁺	2.03e-4	5.39e-4

2.2 Task 2 - Chemistry in quiescent dark clouds

The key theme of this task was to study the chemical composition of quiescent dark interstellar clouds from an evolutionary perspective. Evolutionary chemical models differ from the "classical" fixed physical condition chemical equilibrium models in one extremely important way. The fixed condition equilibrium models assume that the clouds are in equilibrium, so that there is no need to consider the past evolutionary history in deriving the present chemical composition. In the mid-80s, it became quite obvious that the molecular abundances from equilibrium models are at odds with

observations and that it is necessary to consider dynamical evolution in deriving the chemical compositions. This is explained in greater detail in the enclosed reprint.

The present task 2, therefore, has focussed on the chemical composition of gravitationally contracting clouds, because gravitational contraction is one well known means of driving the dynamical evolution of interstellar clouds from their initial diffuse to their final dark cloud state. Two model quiescent, homogeneous and spherical clouds were considered; one with a mass of 40 solar mass and the other with 100 solar mass. The initial densities of both were 100 hydrogen nuclei cm^{-3} . The gravitational contraction of these quiescent interstellar clouds was modeled using the methodology described Prasad, Heere and Tarafdar (*Ap. J.*, 373, 123, 1990) and in the other papers cited by them. The time history of density and temperature in different shells of the contracting clouds were extracted from this calculation. For the chemical calculations at any given evolutionary epoch, the clouds were divided into several concentric shells. The shells were so chosen that the variations of density and temperatures in the adjoining shells were no more than a factor of two. The gravitational contraction was followed until the cloud core reached high density needed for star formation.

Chemical evolution in the two clouds were then modeled separately. The chemical calculations included molecules containing H, C, N, O, S and Si atoms. These modeling were also done by methods described in the above quoted reference.

The present modeling are advances over the previous modeling whose methodology and principles are used. These are advances in the sense that: (i) the use of PAHs, or polycyclic aromatic hydrocarbons, and Si, and (ii) finer gridding of the cloud's spatial domain. The inclusion of PAHs is significant because it helps to increase the availability of neutral carbon atoms and decreases electron density which then promotes molecular growth by suppressing dissociative recombination. The inclusion of Si is important because there are some unresolved problems in the chemistry of the observed silicon bearing molecules that may benefit from evolutionary models. Finer gridding of the cloud helps in better understanding of the spatial variations of the molecules found in the core region.

2.2.2 Preliminary Results

The results of the calculations are being studied. As with the results from the Task 1, it will be quite a while before the full

impact of the results from these evolutionary models can be fully assessed.

In the meantime, Table 2 presents some interesting conclusions from a quick look at the model results for a gravitationally contracting cloud of 100 solar mass. The results shown in Table 2 are for the epoch when the cloud has developed a cold dense core.

Table 2. Model predictions for the densities of various species in a gravitationally contracting cloud of 100 solar mass with and without the PAH's chemistry.

Species	Densities when PAH's chemistry is included	Densities without including PAH's chemistry
Electrons	2.1e-3	4.0e-3
C	3.3e1	1.2e1
CO	3.3e2	3.6e2
C ₂ H	1.6e-4	3.5e-6
C ₃	4.2e-8	4.2e-9
HC ₃ N	1.0e-4	1.4e-5
C ₅	1.0e-8	3.8e-10
HC ₅ N	2.5e-5	8.5e-7
O	4.4e2	4.4e2
O ₂	6.5e1	5.7e1
OH	1.9e-4	1.e-4
H ₂ O	2.4e1	2.5e1
NO	3.0e-4	2.4e-4

The introduction of PAH's chemistry results in a clear decrease of the electron density and a clear increase in the densities of atomic carbon and carbon chain molecules. The electron densities decreases, because electrons can now bind themselves to PAH to form negatively charged PAH⁻. The overall density of positively charged atomic and molecular ion species also decreases

in models that include PAH. This happens because the mutual neutralization of ions is a more efficient process than the radiative recombination of atomic ions, and in some cases than the dissociative recombination also. These results from the models with PAH's chemistry are in better accord with observations and with other contemporary models also. These points will be discussed later in literature publications on which CRE will be concentrating from now onward.

3. CONCLUDING REMARKS:

3.1 ACHIEVEMENTS TO DATE:

Evolutionary modeling of interstellar chemistry was the main thrust of the work done under the subject LMSC P.O., and the parent NASA contract and grant respectively to LMSC and Univ. of Southern California. We have come a long way in this direction. Advantages of our evolutionary modeling, explained in the enclosed reprints of journal papers and conference proceedings, has begun to get recognition in the astrochemistry community. This was most apparent at the IAU Symposium # 150 held on Aug. 5-9, 1991. One of the participant commented: " The idea of Prasad et al that magnetic field can produce such "turning" made out of the core region, thus renewing the chemistry, also produces flatter density distribution with radius that can hydrostatic equilibrium or most dynamical collapse models. Such flatter distribution is precisely what is needed to explain the C¹⁸O observations of these cold dense clouds." (B. E. Turner in Astrochemistry of Cosmic Phenomena, P. D. Singh Ed., Kluwer Academic Pub., p. 210). Summarizing the proceedings, Prof. D. A. Williams, the new Chairman of the Astrochemistry Working Group, emphasized that dynamics must not be ignored, and went further to note the work done under this NASA grant and contract (p. 466 of the above quoted symposium proceedings).

3.2 FUTURE PLANS:

However, the work done so far is just the beginning. Much research work remains to be done to fully exploit the potential of evolutionary models. As far as humanly possible, CRE will continue to work in on this new frontier till a sponsor is found.

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